L-Proline, 1-(trimethylsilyl)-, trimethylsilyl ester

Other names: Proline, 1-(trimethylsilyl)-, trimethylsilyl ester, L-
N,O-Bis-(trimethylsilyl)proline
Proline, N,O-TMS
Proline, di-TMS
Pro, di-TMS
Pro, TMS
Proline, TMS
L-proline, 2tms derivative

Inchi: InChI=1S/C11H25NO2Si2/c1-15(2,3)12-9-7-8-10(12)11(13)14-16(4,5)6/h10H,7-9H2,1-6H

InchiKey: DKGIXVJPGFXLRM-UHFFFAOYSA-N

Formula: C11H25NO2Si2

SMILES: C[Si](C)(C)OC(=O)C1CCCN1[Si](C)(C)C

Mol. weight [g/mol]: 259.49

CAS: 7364-47-8

Physical Properties

Property code	Value	Unit	Source
log10ws	2.03		Crippen Method
logp	2.664		Crippen Method
rinpol	1304.19		NIST Webbook
rinpol	1308.31		NIST Webbook
rinpol	1316.04		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1296.99		NIST Webbook
rinpol	1293.80		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1308.31		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1293.80		NIST Webbook
rinpol	1302.00		NIST Webbook
ripol	1396.61		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7364478&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
ripol:	Polar retention indices